

PROJECT NUMBER: 2520
PROJECT TITLE: Flavor Research
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I. COMMERCIALIZATION OF GMC AND POLYMIC

- A. Objective: To find chemical manufacturers who are capable of producing large quantities of GMC and polyMIC.
- B. Results: GMC produced by John Paine from menthylchloroformate (MCF) in toluene has been found acceptable both analytically and subjectively. Accordingly, a production run of MCF from 1821 pounds of -menthol was carried out by PPG and the material shipped as a toluene solution to Lee Labs. The solution was found analytically acceptable; about 1610 pounds of MCF were produced.

A trial production of 250 pounds of GMC at Lee Labs was begun on November 12. An unanticipated operational failure rendered the entire batch unsuitable for use. Following careful review of all procedures, a second trial will begin during the week of November 26. This material will be available in the first week of December.

II. FLAVOR RELEASE TECHNOLOGY

- A. Objective: To investigate the synthesis and pyrolysis of various flavor release systems for use in new or improved products.
- B. Results: In collaboration with Project 2500 (J. Paine and C. Howe), a large scale preparation of CR-2852 was accomplished. The material (15g) was submitted to Flavor Development for further evaluation as a vanillin sidestream flavoring agent. This large scale preparation was accomplished by two separate routes: one utilized a THP-protected vanillin and the other a benzyl-protected vanillin. Each was condensed with ethyl phenylacetate to yield the corresponding protected hydroxy-esters, which were subsequently de-blocked to give CR-2852. An attempt to carry out a direct large-scale synthesis by condensation of ethyl phenylacetate with unprotected vanillin failed to give the desired product.

An alternate vanillin-release agent (CR-2887) is now available for evaluation by Flavor Development. This compound, a vanillin ester of CR-1719, upon pyrolysis at 300° cleanly yields vanillin and a tobacco-identical lactone. A patent disclosure discussing these results has been submitted.

The preparation of a vanillin ester of gluconic acid continues to provide synthetic challenges. Reaction of di-isopropylidene gluconic acid with vanillin under various conditions failed to

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give any of the desired ester. In the belief that the alpha-hydroxyl group may be interfering with esterification, blocking groups for this free hydroxyl are being investigated.

The analysis of mainstream, sidestream and butts from cigarettes (heavy paper, code X8D9DAU) made from paper coated with Aromatek 245 has been completed. Total accountability of mass was 65%. The amount of Aromatek 245 decomposing to deliver alpha-hexylcinnamaldehyde as well as the distribution of the compounds to MS and SS were nearly identical to that found in a previous study using Marlboro Lights. The sidestream contained 90% of the released aldehyde as well as 80% of the recovered (intact) Aromatek 245.

III. FLAVOR CHEMISTRY

- A. Objective: To obtain flavors for subjective evaluation and odor profiling. To isolate and identify tobacco components which are sensorially significant.
- B. Results: Data from the newly-established Trigeminal panel have been analyzed and the following conclusions drawn:
 - 1. The data are adequately reproducible;
 - 2. The descriptors being used can separate olfactory and trigeminal stimulants clearly;
 - 3. The descriptors can separate Trigeminal stimulants such as nicotine, acetic acid and menthol;

A memo describing these results in greater detail is in preparation. Evaluation of other stimulants continues.

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